Dibenzepin M(Nor), acetylated

Inchi: InChI=1S/C19H21N3O2/c1-14(23)20(2)12-13-22-18-11-7-6-10-17(18)21(3)16-9-5-4-8-15
InchiKey: ZDAPGODXDLFVIH-UHFFFAOYSA-N
Formula: C19H21N3O2
SMILES: CC(=O)N(C)CCN1C(=O)c2ccccc2N(C)c2ccccc21
Mol. weight [g/mol]: 323.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	2.893		Crippen Method
mcvol	253.270	ml/mol	McGowan Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310868&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.